LBNL-62595

Mass- and Temperature-Dependent Diffusion Coefficients for Light Noble Gases for the TOUGH2-EOSN Module

J. L. Andrews
Department of Geology and Geophysics, University of Minnesota
310 Pillsbury Dr. SE
Minneapolis, MN 55455, USA.
andre345@umn.edu

S. Finsterle
Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, California, USA

M. O. Saar
Department of Geology and Geophysics,
University of Minnesota, Minneapolis, Minnesota, USA

April 2007

This work was supported, in part, by the University of Minnesota, George and Orpha Gibson Endowment, and by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

DISCLAIMER

1. INTRODUCTION

This report describes modifications made to the EOSN module (Shan and Pruess, 2003) of the nonisothermal multiphase flow simulator TOUGH2 (Pruess et al., 1999). The EOSN fluid property module simulates transport of water, brine, air, and noble gases or CO_2 in the subsurface. In the standard version of the EOSN module, diffusion coefficients can be specified by the user, but there is no allowance for liquid-phase diffusion coefficients to change with temperature. Furthermore, users must specify radiogenic sources of heat and helium for each element in data block GENER, which can be a time-consuming task for models with large numbers of elements. Our modifications seek to increase the functionality and efficiency of using TOUGH2-EOSN by allowing for mass- and temperature-dependent liquid-phase diffusion coefficients for helium and neon and specification of radiogenic heat and helium production as a property of a material.

The modified version is based on TOUGH2-EOSN and thus requires familiarity with the capabilities and input formats of the TOUGH2 code (Pruess et al., 1999) and the EOSN module (Shan and Pruess, 2003). This report only details our modifications and how to properly utilize them.

2. LIQUID-PHASE DIFFUSION COEFFICIENTS FOR HELIUM AND NEON

A method for calculating temperature- and mass-dependent liquid-phase diffusion coefficients is adopted for the two light noble gases helium and neon. As with the previous version of EOSN, when the DIFFU block is implemented, diffusion coefficients for all five components in both the gas (1,K) and liquid (2,K) phases must be specified (Pruess et al., 1999). The options for temperature- and mass-dependent diffusion coefficients are invoked by specifying a non-zero value FDDIAG(3,K) in columns 21–30 (Figure 1) of data block DIFFU.3 (for noble gas No. 1; for example ^{3}He) and DIFFU.4 (for noble gas No. 2; for example ^{4}He). If FDDIAG(3,K) = 0.0 or is left blank, the diffusion coefficient is constant as specified by the user in data block FDDIAG(2,K). In the case of the light noble gases He and Ne, the diffusion coefficient for the liquid phase is merely a placeholder when FDDIAG(3,K) ≠ 0.0; the value in FDDIAG(2,K) will not be used; instead, the internally calculated temperature-dependent diffusivities are applied. If the gas is not He or Ne, the liquid-phase diffusivity is constant and equal to the diffusivity entered into FDDIAG(2,K), i.e., the column for the liquid-phase diffusivity.

```
NOBLE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
He                3.
He                4.

DIFFU----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
       0.0       0.0
       0.0       0.0
     1.e-9     1.e-9      1.13
     1.e-9     1.e-9      1.00
     1.e-9     1.e-9
```

Figure 1: Modification to data block DIFFU to invoke temperature- and mass-dependent diffusion coefficients for the light noble gases helium and neon

2.1 Temperature-Dependent Liquid Diffusion Coefficient

Temperature-dependent diffusion coefficients are calculated using the following equations from Jähne et al. (1987),

$$D(\mathrm{He})\ [\mathrm{m^2/s}] = 8.180\times10^{-7} \times \exp(-1407 / T) \tag{1}$$

$$D(\mathrm{Ne})\ [\mathrm{m^2/s}] = 1.608\times10^{-6} \times \exp(-1785 / T) \tag{2}$$

where T is temperature in Kelvin. Figure 2 shows the temperature-dependent diffusivities for He and Ne.

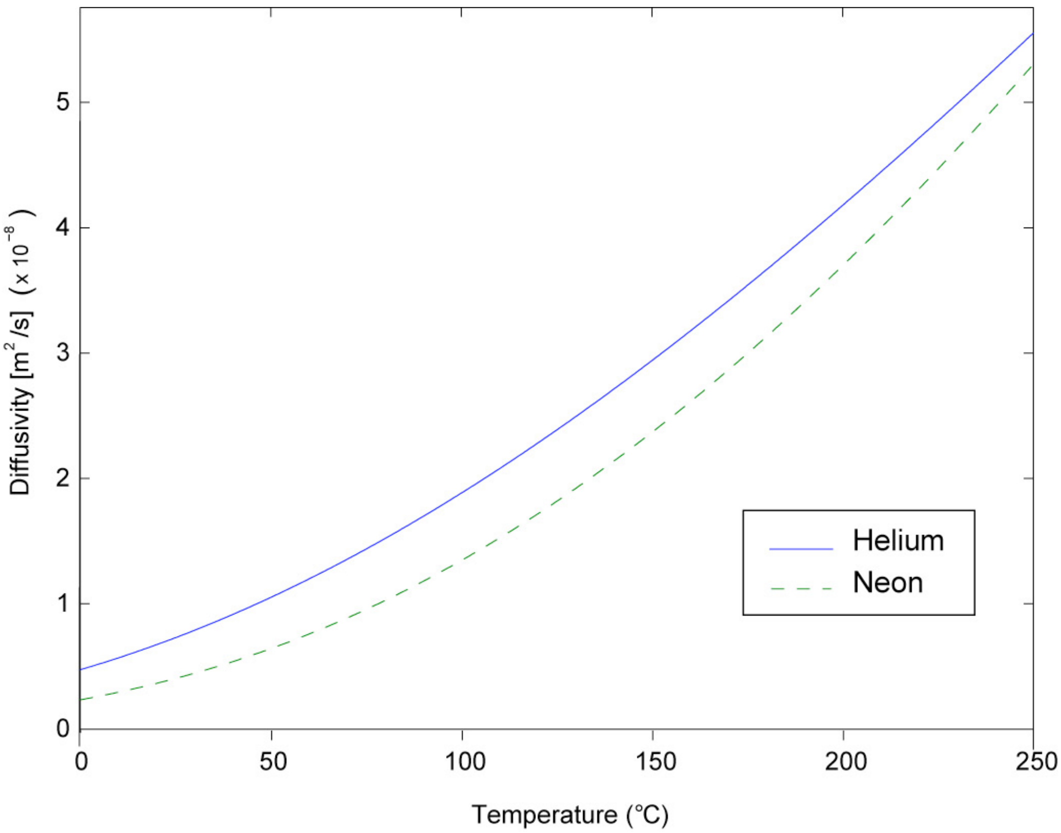

Figure 2: Temperature-dependent liquid-phase diffusivities for helium and neon (Jähne et al., 1987).

During the calculation of mass balances at each time step, the diffusion coefficients are recalculated as a function of the temperature in each element. The code automatically determines whether the noble gas is helium or neon, then uses the appropriate equation to calculate the diffusivity.

2.2 Mass-Dependent Liquid-Phase Diffusion Coefficient

Mass-dependency of the diffusion coefficients can also be considered when implementing temperature-dependence. In this case, the diffusivity is merely a scaled version of the one calculated internally. The diffusion coefficient (DICO) of the noble gas (K) is calculated in the following manner:

$$\mathrm{DICO(K)} = \mathrm{FDDIAG(3,K)} \times D_e(\mathrm{K}) \quad (\mathrm{K}=3,4)\ , \tag{3}$$

where D_e(K) is the effective diffusion coefficient calculated by TOUGH2 using the temperature-dependent equations provided above. The use of FDDIAG(3,K) as a multiplier allows the user to scale the diffusivity to a higher or lower value to include factors such as mass-dependency.

3. RADIOGENIC HEAT AND HELIUM PRODUCTION

Crustal production of heat and ^{4}He is a result of radioactive decay of the uranium and thorium present in the host rock. While some ^{3}He is produced through radiogenesis, the amount created is very small compared to the production of ^{4}He, such that radiogenic production of ^{3}He can often be ignored (Ozima and Podosek, 2002). Because of the unique isotopic signature created by this process, simulation of radiogenic heat and helium production can be useful in determining groundwater flow paths.

With the modified version of TOUGH2-EOSN, radiogenic heat and ^{4}He production can be defined for a material, dispensing of the need to include separate source terms for each element within the domain. There are three blocks of the input file necessary to use this option (Figure 3).

```
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
ROCK1    2   2500.0        0.10   1.0e-18   1.0e-18   1.0e-18       2.5    1000.0
                                                                          -.1e-6

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

NOBLE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
He                3.
He                4.
```

Figure 3: Modification to data block ROCKS1.1 – automatic generation of radiogenic heat and ^{4}He.

(1) ROCKS.1.1 Format (8E10.4). Extended to include the new input variable, HE4P, in columns 71–80. Radiogenic ^{4}He and heat production can be initiated by either specifying a value for the volumetric mass rate of ^{4}He production, or by specifying the volumetric heat production:

HE4P > 0: ^{4}He production rate, Q_{4He} [kg s^{-1} m^{-3}]; the corresponding heat production is calculated internally

HE4P < 0: Volumetric heat production rate, Q_{RHP} [W m^{-3}]; the corresponding ^{4}He production rate is calculated internally

The use of the ROCKS block to simulate radiogenic heat and helium production does not allow for transient production. Generation will remain constant for the duration of the simulation.

(2) The GENER block must be present in the input file for the calculation of generation rates in the simulation. If no other sinks or sources are specified, an empty block must be provided.

(3) Both lines in block NOBLE must be used; ^{4}He must be the second of the listed noble gases.

The value of heat and ^{4}He production rates can be verified by examining the sinks/sources section of the output file. Radiogenic source terms are indicated by Type = RHP (for Radiogenic Heat Production, Figure 4).

```
         TOUGH2-EOSN: EXAMPLE PROBLEM

                                                                             KCYC =   51  -  ITER =    1  -  TIME =0.439805E+20

 ELEMENT SOURCE INDEX      GENERATION RATE     ENTHALPY    FF(GAS)      FF(LIQ.)      P(WB)
                             (KG/S) OR (W)     (J/KG)                                 (PA)

  A21 1   RHP 1    1          0.605030E-15   0.165280E+15
  A31 1   RHP 1    2          0.605030E-15   0.165280E+15
  A41 1   RHP 1    3          0.605030E-15   0.165280E+15
  A51 1   RHP 1    4          0.605030E-15   0.165280E+15
  A61 1   RHP 1    5          0.605030E-15   0.165280E+15
  A71 1   RHP 1    6          0.605030E-15   0.165280E+15
  A81 1   RHP 1    7          0.605030E-15   0.165280E+15
  A91 1   RHP 1    8          0.605030E-15   0.165280E+15
```

Figure 4. Example of TOUGH2 output file showing radiogenic source terms.

Currently, the relationship between heat and ^{4}He production is hard-wired into the code, and is expressed as (Ballentine and Burnard, 2002):

$$Q_{RHP}/Q_{4He} = 1.6528 \times 10^{-14} \text{ [J/kg]} \quad (4)$$

When the user specifies a ^{4}He production rate, that value is multiplied by the volume of rock (V_{Rock} = (1 - porosity) × $V_{Element}$) to obtain a generation rate in [kg/s]. When the user specifies a heat production rate, the above relationship between radiogenic heat and helium production is used to infer the mass of ^{4}He production. In either case, Q_{RHP}/Q_{4He} is added to the element source term as the enthalpy of the injected mass.

4. CODE MODIFICATIONS

The following files and subroutines were changed to implement mass- and temperature-dependent noble gas diffusivity.

File:	eosn.f	
Subroutines:	INPUT	Read new inputs
	MULTI	Calculate diffusivities and radiogenic heat and ^{4}He production
	RFILE	Create radiogenic heat and ^{4}He sources; subroutine added to eosn.f; to overwrite subroutine RFILE in t2f.f)
File	T2	Common blocks added to allow eosn.f to be compiled with t2cg22.f: COMMON/GD1/DIFG1(MNEL) COMMON/GD2/DIFG2(MNEL) COMMON/GD3/DIFG3(MNEL)

5. CODE DEMONSTRATION

We demonstrate the changes made to TOUGH2-EOSN with an example problem simulating heat and helium transport through a simplified cross section of an active geothermal region. Heat and helium from a cooling and degassing magma body enter the base of the reservoir. Elevated helium isotope ratios $R={}^3He/{}^4He$ indicate magmatic influences ($R_m \approx 8\times10^{-6}$), while a lower ratio ($R_a \approx 1.4\times10^{-6}$) is assigned to the top elements, representing surface conditions.

The first portion of the example shows how to implement mass- and temperature-dependent diffusion coefficients for ^3He and ^4He. In the second portion, we make use of the material-specific radiogenic heat and helium production to see how isotopic ratios are affected by the increase in ^4He throughout the system. The input file provided in Figure 5 contains all of the necessary input except for mesh generation.

We start by creating a 10×10-element X-Z mesh with 100-meter grid spacing using MESHMAKER. To maintain constant-value (Dirichlet) boundary conditions along the top of the domain, the file MESH is modified such that the upper elements (A11*) are assigned zero volumes and made inactive. We specify a 10% pressure head gradient, such that groundwater recharge and discharge occur through the left and right portions of the upper model boundary, respectively. Standard mass fraction values of ^3He and ^4He for air-saturated water at 10°C are specified at the top. Along the bottom elements, we employ constant-flux (Neumann) boundary conditions by adding source terms in the GENER data block. Mass- and temperature-dependent diffusion coefficients are specified by assigning non-zero values to FDDIAG(3,3) for both isotopes. FDDIAG(3,3) is set to 1.13 so that ^3He diffusivity is 13% higher than ^4He diffusivity, as suggested by Jähne et al. (1987).

Figure 6 shows the results of the simulations. For comparison, we also provide the results of the same problem using the original EOSN module with a constant diffusion coefficient ($D = 10^{-9}$ m^2/s). With maximum temperatures of 100°C at the base of the model, the inclusion of temperature-dependent diffusion coefficients greatly modifies mass fractions and isotopic ratios. The simulation of radiogenic heat and helium production throughout the system is invoked by the simple change in the input file (see bottom part of Figure 5). Isotopic ratios are lowered throughout the system due to the generation of radiogenic helium.

```
TOUGH2-EOSN with temperature- and mass-dependent diffusivities
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
ROCK1          2500.       .10    1.E-18    1.E-18    1.E-18       2.0     1000.

MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    5    6    2    8
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   2 500      200000000 0001  03 000   0
                       1.E6                          9.81        4.
    1.E-06       1.0
               1.E5              0.            .788E-17            .773E-11
                0.0             10.
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
AA1 1  Q 1    9    1    1          HEAT      2000.
AA1 1 H3 1    9    1    1          COM3     .5E-19
AA1 1 H4 1    9    1    1          COM4     .8E-14

INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1                       .10
          .103195E07              0.0            .788E-17            .773E-11
                0.0              10.0
A11 2                       .10
          .933850E06              0.0            .788E-17            .773E-11
                0.0              10.0
A11 3                       .10
          .835750E06              0.0            .788E-17            .773E-11
                0.0              10.0
A11 4                       .10
          .737650E06              0.0            .788E-17            .773E-11
                0.0              10.0
A11 5                       .10
          .639550E06              0.0            .788E-17            .773E-11
                0.0              10.0
A11 6                       .10
          .541450E06              0.0            .788E-17            .773E-11
                0.0              10.0
A11 7                       .10
          .443350E06              0.0            .788E-17            .773E-11
                0.0              10.0
A11 8                       .10
          .345250E06              0.0            .788E-17            .773E-11
                0.0              10.0
A11 9                       .10
          .247150E06              0.0            .788E-17            .773E-11
                0.0              10.0
A1110                       .10
          .149050E06              0.0            .788E-17            .773E-11
                0.0              10.0

DIFFU----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
       0.0       0.0
       0.0       0.0
     1.e-9     1.e-9      1.13
     1.e-9     1.e-9      1.00
     1.e-9     1.e-9
NOBLE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
He                3.        0. 0
He                4.        0.

ENDCY

To implement RHP:
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
ROCK1    1     2500.       .10    1.E-18    1.E-18    1.E-18       2.0     1000.
                                                                          -.1e-6
```

Figure 5: TOUGH2 input for example problem

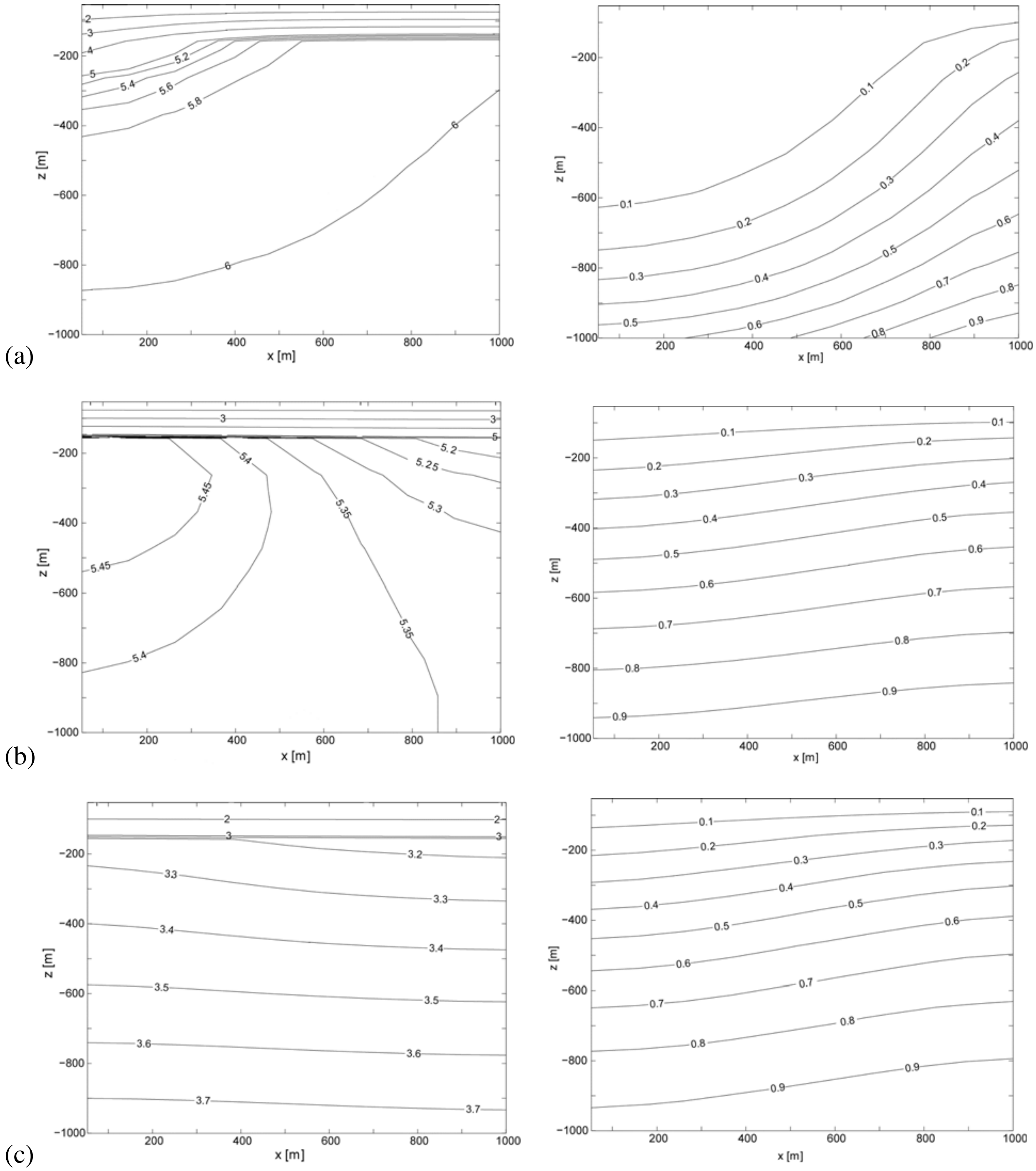

Figure 6: Simulation results for (a) constant diffusion coefficients (standard TOUGH2-EOSN), (b) mass- and temperature-dependent diffusion coefficients, no radiogenic production, (c) mass- and temperature-dependent diffusion coefficients, with radiogenic production. [left]: R/R_a;[right]: mass fraction of ^{4}He, normalized to maximum value. Groundwater recharge occurs at the upper left side of the model; discharge at the upper right side.

```
TOUGH2-EOSN with temperature- and mass-dependent diffusivities

         OUTPUT DATA AFTER (   51,  1)-2-TIME STEPS                                                       THE TIME IS 0.509033E+15 DAYS

 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

  TOTAL TIME     KCYC   ITER  ITERC    KON         DX1M         DX2M         DX3M         MAX. RES.      NER    KER        DELTEX
 0.439805E+20     51      1    119      2       0.00000E+00  0.00000E+00  0.00000E+00    0.44961E-06      46      6       0.87961E+19

 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@


 ELEM.  INDEX      P            T           SL       XBRINE(LIQ)  XNG1(LIQ)   XNG2(LIQ)    XAIRG      XNG1(GAS)   XNG2(GAS)      DL
                  (PA)       (DEG-C)                                                                                          (KG/M**3)

 A21 1      1 0.18269E+07 0.20000E+02 0.10000E+01 0.00000E+00 0.87583E-15 0.25982E-09 0.00000E+00 0.53642E-08 0.15914E-02 0.99911E+03
 A31 1      2 0.27033E+07 0.30001E+02 0.10000E+01 0.00000E+00 0.18810E-14 0.54472E-09 0.00000E+00 0.64562E-08 0.18697E-02 0.99690E+03
 A41 1      3 0.36187E+07 0.40003E+02 0.10000E+01 0.00000E+00 0.29098E-14 0.82762E-09 0.00000E+00 0.57282E-08 0.16293E-02 0.99383E+03
 A51 1      4 0.45539E+07 0.50006E+02 0.10000E+01 0.00000E+00 0.38952E-14 0.10888E-08 0.00000E+00 0.44943E-08 0.12563E-02 0.99001E+03
 A61 1      5 0.54989E+07 0.60008E+02 0.10000E+01 0.00000E+00 0.48043E-14 0.13196E-08 0.00000E+00 0.33156E-08 0.91071E-03 0.98555E+03
 A71 1      6 0.64480E+07 0.70011E+02 0.10000E+01 0.00000E+00 0.56251E-14 0.15178E-08 0.00000E+00 0.23670E-08 0.63869E-03 0.98051E+03
 A81 1      7 0.73977E+07 0.80013E+02 0.10000E+01 0.00000E+00 0.63574E-14 0.16848E-08 0.00000E+00 0.16611E-08 0.44020E-03 0.97496E+03
 A91 1      8 0.83458E+07 0.90014E+02 0.10000E+01 0.00000E+00 0.70066E-14 0.18234E-08 0.00000E+00 0.11563E-08 0.30093E-03 0.96894E+03
 AA1 1      9 0.92907E+07 0.10001E+03 0.10000E+01 0.00000E+00 0.75793E-14 0.19368E-08 0.00000E+00 0.80300E-09 0.20520E-03 0.96248E+03
 A21 2     10 0.17862E+07 0.20000E+02 0.10000E+01 0.00000E+00 0.93903E-15 0.27969E-09 0.00000E+00 0.57504E-08 0.17128E-02 0.99909E+03
 A31 2     11 0.26826E+07 0.30002E+02 0.10000E+01 0.00000E+00 0.19539E-14 0.56732E-09 0.00000E+00 0.67057E-08 0.19470E-02 0.99690E+03
 A41 2     12 0.36065E+07 0.40004E+02 0.10000E+01 0.00000E+00 0.29767E-14 0.84802E-09 0.00000E+00 0.58596E-08 0.16693E-02 0.99382E+03
 A51 2     13 0.45461E+07 0.50007E+02 0.10000E+01 0.00000E+00 0.39521E-14 0.11059E-08 0.00000E+00 0.45597E-08 0.12759E-02 0.99001E+03
 A61 2     14 0.54936E+07 0.60009E+02 0.10000E+01 0.00000E+00 0.48509E-14 0.13333E-08 0.00000E+00 0.33477E-08 0.92011E-03 0.98555E+03
 A71 2     15 0.64442E+07 0.70011E+02 0.10000E+01 0.00000E+00 0.56629E-14 0.15287E-08 0.00000E+00 0.23829E-08 0.64325E-03 0.98051E+03
 A81 2     16 0.73948E+07 0.80013E+02 0.10000E+01 0.00000E+00 0.63884E-14 0.16936E-08 0.00000E+00 0.16691E-08 0.44248E-03 0.97496E+03
 A91 2     17 0.83434E+07 0.90015E+02 0.10000E+01 0.00000E+00 0.70329E-14 0.18308E-08 0.00000E+00 0.11606E-08 0.30214E-03 0.96894E+03
 AA1 2     18 0.92886E+07 0.10002E+03 0.10000E+01 0.00000E+00 0.76033E-14 0.19435E-08 0.00000E+00 0.80553E-09 0.20591E-03 0.96248E+03
 A21 3     19 0.17292E+07 0.20001E+02 0.10000E+01 0.00000E+00 0.10291E-14 0.30785E-09 0.00000E+00 0.63003E-08 0.18848E-02 0.99906E+03
 A31 3     20 0.26483E+07 0.30003E+02 0.10000E+01 0.00000E+00 0.20732E-14 0.60412E-09 0.00000E+00 0.71138E-08 0.20729E-02 0.99688E+03
 A41 3     21 0.35849E+07 0.40005E+02 0.10000E+01 0.00000E+00 0.30944E-14 0.88373E-09 0.00000E+00 0.60904E-08 0.17393E-02 0.99381E+03
 A51 3     22 0.45317E+07 0.50008E+02 0.10000E+01 0.00000E+00 0.40558E-14 0.11368E-08 0.00000E+00 0.46788E-08 0.13114E-02 0.99000E+03
 A61 3     23 0.54837E+07 0.60010E+02 0.10000E+01 0.00000E+00 0.49376E-14 0.13586E-08 0.00000E+00 0.34072E-08 0.93753E-03 0.98554E+03
 A71 3     24 0.64370E+07 0.70013E+02 0.10000E+01 0.00000E+00 0.57338E-14 0.15491E-08 0.00000E+00 0.24126E-08 0.65179E-03 0.98051E+03
 A81 3     25 0.73893E+07 0.80014E+02 0.10000E+01 0.00000E+00 0.64468E-14 0.17101E-08 0.00000E+00 0.16843E-08 0.44678E-03 0.97495E+03
 A91 3     26 0.83388E+07 0.90016E+02 0.10000E+01 0.00000E+00 0.70827E-14 0.18448E-08 0.00000E+00 0.11688E-08 0.30444E-03 0.96893E+03
 AA1 3     27 0.92844E+07 0.10002E+03 0.10000E+01 0.00000E+00 0.76487E-14 0.19562E-08 0.00000E+00 0.81031E-09 0.20724E-03 0.96248E+03
 A21 4     28 0.16648E+07 0.20002E+02 0.10000E+01 0.00000E+00 0.11376E-14 0.34179E-09 0.00000E+00 0.69632E-08 0.20920E-02 0.99903E+03
 A31 4     29 0.26060E+07 0.30005E+02 0.10000E+01 0.00000E+00 0.22239E-14 0.65047E-09 0.00000E+00 0.76287E-08 0.22314E-02 0.99686E+03
 A41 4     30 0.35567E+07 0.40007E+02 0.10000E+01 0.00000E+00 0.32479E-14 0.93017E-09 0.00000E+00 0.63913E-08 0.18304E-02 0.99380E+03
 A51 4     31 0.45125E+07 0.50010E+02 0.10000E+01 0.00000E+00 0.41939E-14 0.11778E-08 0.00000E+00 0.48374E-08 0.13585E-02 0.98999E+03
 A61 4     32 0.54701E+07 0.60012E+02 0.10000E+01 0.00000E+00 0.50544E-14 0.13927E-08 0.00000E+00 0.34874E-08 0.96096E-03 0.98553E+03
 A71 4     33 0.64271E+07 0.70014E+02 0.10000E+01 0.00000E+00 0.58302E-14 0.15768E-08 0.00000E+00 0.24529E-08 0.66338E-03 0.98050E+03
 A81 4     34 0.73816E+07 0.80016E+02 0.10000E+01 0.00000E+00 0.65266E-14 0.17327E-08 0.00000E+00 0.17050E-08 0.45266E-03 0.97495E+03
 A91 4     35 0.83324E+07 0.90017E+02 0.10000E+01 0.00000E+00 0.71510E-14 0.18640E-08 0.00000E+00 0.11800E-08 0.30758E-03 0.96893E+03
 AA1 4     36 0.92786E+07 0.10002E+03 0.10000E+01 0.00000E+00 0.77110E-14 0.19736E-08 0.00000E+00 0.81687E-09 0.20908E-03 0.96248E+03
 A21 5     37 0.15969E+07 0.20003E+02 0.10000E+01 0.00000E+00 0.12615E-14 0.38060E-09 0.00000E+00 0.77193E-08 0.23289E-02 0.99900E+03
 A31 5     38 0.25594E+07 0.30006E+02 0.10000E+01 0.00000E+00 0.23962E-14 0.70346E-09 0.00000E+00 0.82176E-08 0.24125E-02 0.99684E+03
 A41 5     39 0.35246E+07 0.40009E+02 0.10000E+01 0.00000E+00 0.34246E-14 0.98348E-09 0.00000E+00 0.67374E-08 0.19349E-02 0.99378E+03
 A51 5     40 0.44901E+07 0.50012E+02 0.10000E+01 0.00000E+00 0.43536E-14 0.12251E-08 0.00000E+00 0.50208E-08 0.14129E-02 0.98998E+03
 A61 5     41 0.54542E+07 0.60014E+02 0.10000E+01 0.00000E+00 0.51902E-14 0.14323E-08 0.00000E+00 0.35807E-08 0.98810E-03 0.98553E+03
 A71 5     42 0.64154E+07 0.70016E+02 0.10000E+01 0.00000E+00 0.59427E-14 0.16090E-08 0.00000E+00 0.25000E-08 0.67686E-03 0.98049E+03
 A81 5     43 0.73725E+07 0.80017E+02 0.10000E+01 0.00000E+00 0.66200E-14 0.17591E-08 0.00000E+00 0.17293E-08 0.45952E-03 0.97494E+03
 A91 5     44 0.83249E+07 0.90018E+02 0.10000E+01 0.00000E+00 0.72311E-14 0.18864E-08 0.00000E+00 0.11932E-08 0.31127E-03 0.96892E+03
 AA1 5     45 0.92717E+07 0.10002E+03 0.10000E+01 0.00000E+00 0.77843E-14 0.19941E-08 0.00000E+00 0.82458E-09 0.21123E-03 0.96247E+03
```

Figure 7: Excerpt from TOUGH2-EOSN output file for the example problem

7. CONCLUSIONS

The modified version of TOUGH2-EOSN presented in this report provides greater functionality for modeling transport of the light noble gases by making available mass- and temperature-dependent diffusion coefficients of helium and neon. It also provides greater efficiency in implementation of radiogenic processes by allowing the user to specify radiogenic heat and ^{4}He production for an entire material according to a volumetric heat or ^{4}He production rate. These changes are shown to have a significant effect on both concentration and isotopic ratio patterns. These new capabilities, therefore, also provide new tools for interpreting aquifer processes for researchers using noble gases as natural tracers of groundwater transport.

ACKNOWLEDGMENT

We would like to thank Yingqi Zhang and Ravi Appana for thoughtful review comments. This work was supported, in part, by the University of Minnesota, George and Orpha Gibson Endowment, and by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

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